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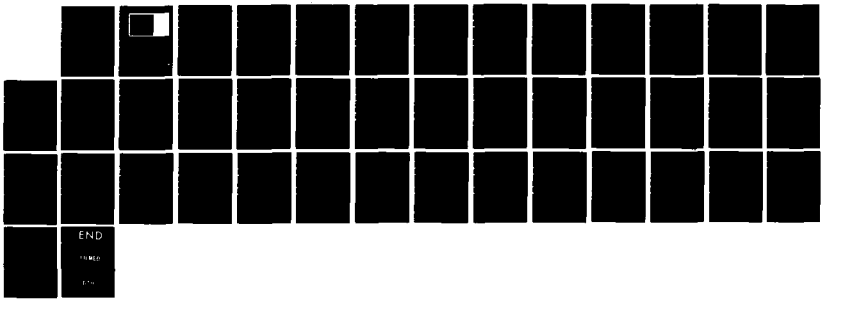

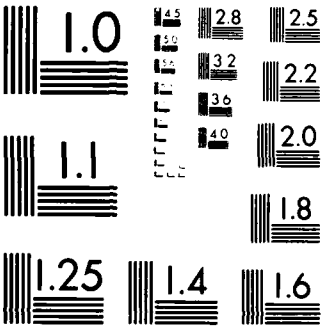

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A SECOND ORDER DIFFERENCE SCHEME FOR TRANSIENT SEMICONDUCTOR DEVICE SIMULATION

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ABSTRACT

A second order scheme for the solution of the transient fundamental semiconductor device equations is presented which does not suffer from timestep restrictions due to the stiffness of the analytical problem. The second order accuracy as well as the stability properties are demonstrated on the simulation of a p-n-junction diode.

AMS (MOS) Subject Classifications: 35G25, 35M05, 65M15

Key Words: Semiconductors, Singular Perturbations, Finite Differences,

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SIGNIFICANCE AND EXPLANATION

In recent years there has been an increasing amount of interest in the calculation of A-C properties of silicon-based semiconductor devices, mainly due to the rapid developments in fabrication technology and the resulting miniaturization. This makes the numerical solution of the so-called transient fundamental semiconductor equations an absolute necessity. Most existing numerical methods for this problem are only first-order accurate in time because of the quite complicated anlaytical structure of the equations ('stiffness'). In this paper we present a new method which is based on an asymptotic analysis of this structure. In contrast to existing methods, it is genuinely of second order and does not suffer from any timestep restrictions. It therefore improves the overall efficiency of A-C calculations significantly compared to the existing methods.

A SECOND ORDER DIFFERENCE SCHEME FOR TRANSIENT SEMICONDUCTOR DEVICE SIMULATION

Christian A. Ringhofer

0. Introduction

In this paper we present a finite difference discretization method for the basic semiconductor device equations in the transient case. These equations - describing the field, carrier - and current concentration in a semiconductor material - are given by (see c.f. Von Roosbroeck [1950])

$$(0.1) \qquad \varepsilon \Delta \Psi = q(n-p-C)$$

$$(0.2) \qquad a) \ \nabla \cdot J_n = q[n_t+R], \quad b) \ \nabla \cdot J_p = -q[p_t+R]$$

$$(0.3) \qquad a) \ J_n = q[D_n \nabla n - \mu_n n \nabla \Psi], \quad b) \ J_p = -q[D_p \nabla p + \mu_p p \nabla \Psi]$$

The independent variables in (0.1) - (0.3) have the following meaning:

Ψ	electric potential
$-\nabla\Psi$	electric field
n	negative (electron-) carrier density
p	positive (hole-) carrier density
J_n	electron current density
J_p	hole current density

ε and q in (0.1) - (0.3) denote the dielectric permitivity and the unit charge and are material constants. D_n, D_p and μ_n, μ_p denote the diffusion coefficients and mobilities of electrons and holes which in general are functions of the electric field $-\nabla\Psi$. It is assumed that Einstein's relation

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(0.4) $\quad D_n = u_T \mu_n \quad , \quad D_p = u_T \mu_p$

holds where u_T - the thermal voltage - is only dependent on temperature and therefor a constant. $C(\vec{x})$ in (0.1) denotes the doping concentration (the preconcentration of electrons and holes in the semiconductor). The regions where $C(\vec{x}) > 0$ and $C(\vec{x}) < 0$ holds are called the n and p regions respectively and the manifolds given by $C(\vec{x}) = 0$ are called the p-n junctions. R in (0.2) - denotes the generation - recombination rate of electrons and holes and will in general be a nonlinear function of n,p and $\nabla\Psi$. (See Sze [1969] or Sellerherr [1984] for different models for R). (0.1) - (0.3) will be subject to the initial conditions

(0.5) $\quad \Psi(\vec{x},0) = \Psi_I(\vec{x}),\ n(\vec{x},0) = n_I(\vec{x}),\ p(\vec{x},0) = p_I(\vec{x})$

where

(0.6) $\quad \varepsilon\Delta\Psi_I = n_I - p_I - C$

has to hold because of compatibility with (0.1). This paper is concerned with the twodimensional model only. So (0.1) - (0.3) will hold for $\vec{x} \in \Omega \subset R^2$. At each point of the boundary $\partial\Omega$ three boundary conditions are imposed which we write in the form

(0.7) $\quad B(\Psi,n,p,\nabla\Psi,J_n,J_p) = b(t) \quad x \in \partial\Omega.$

The shape of Ω and the boundary conditions B will depend on the particular

device under consideration. A typical case is the following:

(0.8) $\partial\Omega = \partial\Omega_1 \cup \partial\Omega_2$

(0.9) a) $\Psi = V(t)$, b) $n - p = n_i^2$, c) $n - p - C = 0$ for $x \in \partial\Omega_1$

(0.10) a) $\nabla\Psi \cdot \vec{n} = 0$, b) $J_n \cdot \vec{n} = 0$, c) $J_p \cdot \vec{n} = 0$ for $x \in \partial\Omega_2$

where $\partial\Omega_1$ represents Ohmic contacts and $\partial\Omega_2$ an insulator. $\vec{n}$ denotes the normal vector on the boundary and n_i is a given constant. V(t) in (0.10) represents the voltage applied to the device which is varied in time. (i.e. the input is 'switched'.)

The scope of this paper is to develop a finite difference method for (0.1) - (0.3) which is second order accurate in time. As shown by Ringhofer [1984] b) the problem is extremely stiff in time and at the same time exhibits an internal layer behavior in the spacial directions. This causes simple one-step methods based on central differencing (i.f. Crank-Nicholson) to suffer from prohibitive timestep restrictions. First we scale the problem appropriately in Sec. 1. Then - by making use of a singular perturbation analysis for the steady state - and the transient problem carried out in Markorwich and Ringhofer [1984], Markorwich [1984] and Ringhofer [1984] b) we develop a discretization scheme which does not suffer from any timestep restrictions and although of first order formally is second order accurate for the range of timesteps one wishes to use in practice. In on unscaled form it is of the form

$$(0.11) \qquad \varepsilon\Delta\psi^{k+1} = q[n^{k+1} - p^{k+1} - C]$$

$$(0.12) \qquad \frac{1}{\Delta t_k}(n^{k+1}-n^k) = \frac{1}{4q}\nabla\cdot[3J_n^{k+1} + J_n^k + J_p^{k+1} - J_p^k] - \frac{1}{2}[R^k + R^{k+1}]$$

$$(0.13) \qquad \frac{1}{\Delta t_k}(p^{k+1}-p^k) = -\frac{1}{4q}[3J_p^{k+1} + J_p^k + J_n^{k+1} - J_n^k] - \frac{1}{2}[R^k + R^{k+1}]$$

$$(0.14) \qquad J_n^\ell = q[D_n^\ell \nabla n^\ell - \mu_n^\ell n^\ell \nabla\psi^\ell] \quad , \quad \ell = k,\ k+1$$

$$(0.15) \qquad J_p^\ell = -q[D_p^\ell \nabla p^\ell + \mu_p^\ell p^\ell \nabla\psi^\ell] \quad , \quad \ell = k,\ k+1$$

where the superscript ℓ denotes a variable at the discrete timelevel t_ℓ and $\Delta t_k = t_{k+1} - t_k$ holds. R^ℓ, D_n^ℓ, μ_n^ℓ e.t.c. denote R, D_n, μ_n e.t.c. with their arguments taken at $t = t_\ell$. The spacial differential operators in (0.11 - (0.15) are discretized by standard exponentially fitted finite differences due to Scharfetter and Gummel [1969]. The spacial discretization is given in Sec. 3. In Sec. 4. the time discretization is derived and an argument is given that (0.11) - (0.15) is second order accurate as long as the timesteps are larger than the dielectric relaxation time. The second order accuracy is verified numerically in Sec. 6.

1. Scaling and Singular Perturbation Formulation

In this section we scale (0.1) - (0.3) appropriately and reformulate it as a singular perturbation problem. We assume

(1.1) $$\mu_n = \mu_p = \mu = \text{const}$$

for this and the next two sections. It should be pointed out that (1.1) is probably a highly unrealistic assumption and therefor inadequate. Assumption (1.1) is only made for the sake of notational simplicity and in Sec. 5. the scaling and the scheme is given for the case of a general model for the mobilities. We scale the independent variables $\vec{x}$ and t to O(1). That means that after scaling the size of Ω and the speed with which V(t) in (0.9) is varied is O(1).

(1.2) $$\vec{x} = \ell \vec{x}_s, \quad t = \ell^2 (u_T \mu)^{-1} t_s$$

Here ℓ denotes some characteristic device length. We scale n and p such that their maximal size at Ohmic contacts is O(1) in (0.9):

(1.3) $$n = \bar{C} n_s, \quad p = \bar{C} p_s, \quad \bar{C} := \max_{\vec{x}} |C(x)|.$$

For ψ, J_n and J_p we use the scaling

(1.4) $$\psi = u_T \psi_s, \quad J_n = q\bar{C} u_T \mu \ell^{-1} J_{n_s}, \quad J_p = q\bar{C} u_T \mu \ell^{-1} J_{p_s}.$$

After scaling (0.1) - (0.3) assumes the form

$$\text{(1.5)} \qquad \lambda^2 \Delta \Psi_s = n_s - p_s - C_s, \quad \left(C_s(\vec{x}) = \frac{C(\vec{x})}{\max_{\vec{x}} |C(\vec{x})|}\right)$$

$$\text{(1.6)} \qquad \text{a)} \quad n_{s_t} = \nabla \cdot J_{n_s} - R_s, \qquad \text{b)} \quad p_{s_t} = - \nabla \cdot J_{p_s} - R_s$$

$$\text{(1.7)} \qquad \text{a)} \quad J_{n_s} = \nabla n_s - n_s \nabla \Psi_s, \qquad \text{b)} \quad J_{p_s} = - \nabla p_s - p_s \nabla \Psi_s.$$

The subscripts s will be ommitted from hereon. The initial and boundary conditions have to be scaled accordingly. λ in (1.5) is a small constant and acts as a singular perturbation parameter.

$$\text{(1.8)} \qquad \lambda = (\varepsilon u_T)^{1/2} \, (q \ell^2 \bar{C})^{-1/2}$$

For practical devices $\lambda << 1$ will hold. (For instance for a 1μ silicon device with a maximal doping $\bar{C} = 10^{19}$ cm^{-3} $\lambda = 0(10^{-3})$ will hold.) λ, which is proportional to the minimal Debey length, has been used as a perturbation parameter in a singular perturbation analysis of (1.5) - (1.7) in the steady state case by Markorwich and Ringhofer [1984] and Markorwich [1984] and for the transient problem by Ringhofer [1984] b). Since we rely heavily on their results for the development of our method we briefly sketch them in the following section.

2. Analytical Results

In this section we discuss some analytical properties of the solution of (1.5) - (1.7). These results will be used in the following sections to motivate the choice of the discretization scheme. We are motivated by a singular perturbation analysis carried out previously for the problem (1.5) - (1.7). We therefor focus on the information about the structure of the solution obtained by this asymptotic analysis. For the precise results as well as the proofs of these results we refer the reader to the corresponding literature. It turns out that the problem (1.5) - (1.7) is singularly perturbed in both the space and the time dimension i.e. the solution exhibits a layer structure in the spacial variables and can evolve on several different timescales simultaneously. Away from $t = 0$ and the layer regions the solution of (1.5) - (1.7) will be given up to terms of order $O(\lambda)$ by the outer solution $\tilde{w} = (\tilde{\psi},\tilde{n},\tilde{p},\tilde{J}_n,\tilde{J}_p)^T$ of

$$(2.1) \qquad 0 = \tilde{n} - \tilde{p} - C$$

$$(2.2) \qquad a)\ \tilde{n}_t = \nabla\cdot\tilde{J}_n - \tilde{R} \quad , \quad b)\ \tilde{p}_t = \nabla\cdot\tilde{J}_p - \tilde{R}$$

$$(2.3) \qquad a)\ \tilde{J}_n = \nabla\tilde{n} - \tilde{n}\nabla\tilde{\psi} \quad , \quad b)\ \tilde{J}_p = -\nabla\tilde{p} - \tilde{p}\nabla\tilde{\psi}.$$

So Poisson's equation degenerates for $\lambda \to 0$ into the condition of vanishing space charge. Because of this drop in order $\tilde{w}$ can not be expected to satisfy all boundary conditions (0.7) automatically. It turns out however that (2.1) is consistent with (0.9) c) and one of the conditions (0.10) a), b) is satisfied automatically as soon as the other one is because $\nabla C\cdot\vec{n} = 0$ holds on the

appropriate parts of the boundary $\partial\Omega$. Therefor all boundary conditions (0.9) - (0.10) can be satisfied by $\tilde{w}$ and no boundary layers occur (see Markowich [1984]). We are confronted however with an internal layer structure around the p-n junctions. The doping profile $C(\vec{x})$ will vary very rapidly across the p-n-junctions and in the extreme case is even modelled as discontinuous there. In either case $\tilde{n}$ and $\tilde{p}$ have to be discontinuous across the p-n-junctions in order to satisfy (2.1) and this causes the 'full' solution w to develop a layer there. Because $\tilde{w}$ is discontinuous (2.2) - (2.3) can not hold at the p-n-junction and the reduced problem has to be supplemented by 4 jump conditions there. These conditions have been derived in Markowich and Ringhofer [1984] and Markowich, Ringhofer et. al. [1983] and are of the form:

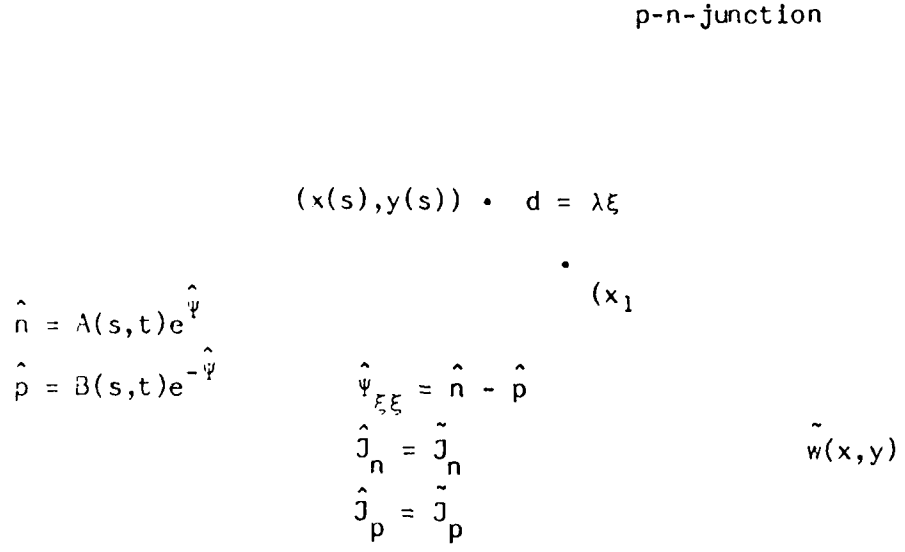
$$(2.4) \qquad ne^{-\Psi},\ pe^{\Psi},\ J_n \cdot \vec{n},\ J_p \cdot \vec{n}$$

are continuous across the p-n-junction where $\vec{n}$ denotes the unit normal vector on the p-n-junction. These conditions say that the currents and the equi-fermi-potentials are preserved across the junctions. Inside the p-n-junction layers Ψ n and p vary in the 'fast' spacial variable $\xi = d/\lambda$ where d denotes the perpendicular distance of a point $\vec{x}$ from the p-n-junction. They are given by $\hat{\Psi}$, $\hat{n}$, $\hat{p}$ satisfying

$$(2.5) \qquad a)\ \hat{n} = A(s,t)e^{\hat{\Psi}}, \qquad b)\ \hat{p} = B(s,t)e^{-\hat{\Psi}}$$

$$(2.6) \qquad \hat{\Psi}_{\xi\xi} = \hat{n} - \hat{p} - C$$

where s is some parametrization of the p-n-junction and A and B are determined by the solution $\tilde{w}$ of the reduced problem (2.1) - (2.4). J_n and J_p do not exhibit any layer behavior. The spacial structure of the solution is depicted graphically in the figure below.



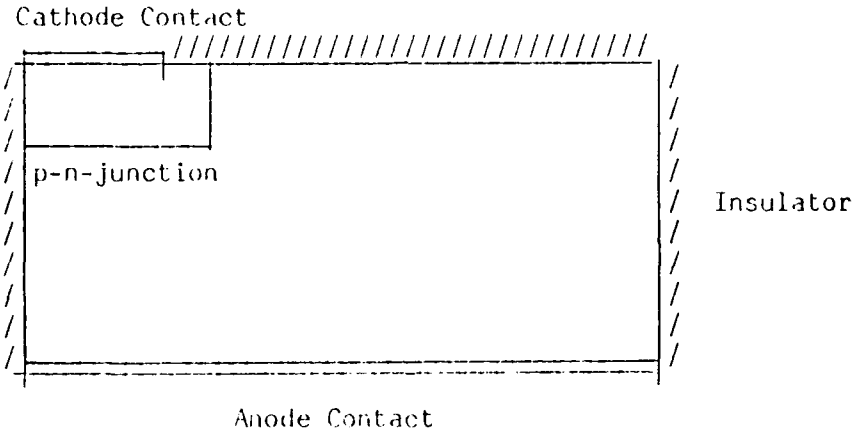
So far we have described the structure of the solution away from t = 0. If the described asymptotic structure is to hold for all t > 0, the initial functions ψ_I, n_I and p_I apparently have to satisfy the relations (2.1) and (2.6). Moreover differentiating (2.1) with respect to t and using (2.2) a) b) yields

$$\nabla \cdot (\tilde{J}_n + \tilde{J}_p) = 0 \tag{2.7}$$

which gives an additional condition on ψ_I, n_I and p_I. In Markowich and Ringhofer [1984] and Markowich [1984] it is shown that these conditions are satisfied if ψ_I, n_I, p_I are the solutions of the steady state problem

6. Numerical Results

In this section we verify the stability and convergence properties of the discussed scheme for the case of a p-n-junction diode. The length and depth of the device are taken to be 1μ and 0.25 μ respectively. The doping profile C is taken to the constant 10^{19} cm^{-3} in the n-region and -10^{15} cm^{-3} in the p-region. (So we consider an abrupt p-n-junction). After employing the scaling of Sec. 1 we obtain the system (1.5) - (1.7) posed on a rectangular domain of the form



The length and width of the domain are 1 and 0.25 respectively. λ turns out to be 5.10^{-3} in this case. The contacts correspond to the part $\partial\Omega_1$ of the boundary. So the boundary conditions (0.9) are imposed there. This insolator corresponds to $\partial\Omega_2$ and (0.10) is imposed on this part of the boundary. The voltage applied to the diode is given by the difference in Ψ between the two contacts calibrated by the built in potential Ψ_{D_i} (see c.f. Sze [1969]). So the boundary condition for Ψ in (0.9) a) assumes the form

(6.1) a) $\Psi(x,t) = \Psi_{D_i}(x) + \frac{1}{2}u(t)$ x at the anode

(5.4) $\lambda^2\Delta\Psi = n - p - C$

(5.5) a) $n_t = \nabla\cdot J_n + R$ b) $p_t = -\nabla\cdot J_p - R$

(5.6) a) $J_n = D_n^S(\nabla n - n\nabla\Psi)$ b) $J_p = -D_p^S(\nabla p + p\nabla\Psi)$

$$D_r^S(x_s,\nabla\Psi_s) = (\overline{\mu}_n\overline{\mu}_p)^{-1/2}\,\mu_r(\ell\vec{x}_s, \frac{u_T}{\ell}\nabla\Psi_s) \quad , \quad r = n,p.$$

To implement (5.4) - (5.6) into the discretization method (4.13) - (4.17), (4.16) - (4.17) has to be replaced by

(5.7) $J_n = D_n^S[\kappa\nabla_h n - (Bn)\nabla_h\Psi]$

(5.8) $J_p = -D_p^S[\kappa\nabla_h p + (Bp)\nabla_h\Psi]$

$$D_{r_{ij}}^S := D_r^S(x_{ij},\nabla_h\Psi_{ij}) \quad , \quad r = n,p$$

5. Variable Mobilities

As mentioned in Sec. 1 the assumption $\mu_n = \mu_p = \text{const}$ and $D_n = D_p = \text{const}$ is quite unrealistic. As pointed out in Mock [1981] it might sometimes be justifyable in steady state simulations while it is probably inadequate in the transient case. It is however reasonable to assume that Einstein's relation

$$\frac{D_n}{\mu_n} = \frac{D_p}{\mu_p} = u_T \tag{5.1}$$

holds where u_T only depends on temperature (and therefore is constant for our purposes). Various models for μ_n and μ_p have been proposed (see c.f. Selberherr [1984] for an overview). In the most general case μ_n and μ_p will depend on $\vec{x}$ and on the electric field - $\nabla\psi$ i.e.

$$\mu_r = \mu_r(\vec{x}, \nabla\psi), \quad D_r = u_T\mu_r, \quad r = n,p \tag{5.2}$$

To include this form of the parameters D_n, D_p, μ_n and μ_p into the model the scaling has to be slightly modified first: μ_n and μ_p are scaled by some characteristic values $\bar{\mu}_n$ and $\bar{\mu}_p$ t, J_n and J_p are then scaled by

$$t = \ell^2\bar{D}^{-1}t_s, \quad J_n = \bar{D}\bar{C}\ell^{-1}J_{n_s}, \quad J_p = \bar{D}\bar{C}\ell^{-1}J_{p_s}$$

$$\bar{D} = u_T(\bar{\mu}_n\bar{\mu}_p)^{1/2} \tag{5.3}$$

(1.5) - (1.7) then becomes

(4.10) in the given form since it involves a fourth order difference operator in space and it is difficult to implement nonconstant mobilities μ_n and μ_p in this form. We therefor rewrite (4.7) - (4.10) using the original variable set $(\psi,n,p,J_n,J_p)^T$ and obtain

$$\lambda^2 \operatorname{div}_h \nabla_h \psi^{k+1} = n^{k+1} - p^{k+1} - C \tag{4.13}$$

$$\frac{1}{\Delta t_k}(n^{k+1}-n^k) = \frac{1}{4}\left[\operatorname{div}_h(3J_n^{k+1} + J_n^k + J_p^{k+1} + J_p^k) - 2R^k - 2R^{k+1}\right] \tag{4.14}$$

$$\frac{1}{\Delta t_k}(p^{k+1}-p^k) = -\frac{1}{4}\left[\operatorname{div}_h(3J_p^{k+1} + J_p^k + J_n^{k+1} - J_n^k) + 2R^k + 2R^{k+1}\right] \tag{4.15}$$

$$J_n^\ell = \left[\kappa^\ell \nabla_h n^\ell - (\mu n^\ell)\nabla_h \psi^\ell\right] \tag{4.16}$$

$$\ell = k,\ k+1$$

$$J_p^\ell = \left[\kappa^\ell \nabla_h p^\ell + (\mu p^\ell)\nabla_h \psi^\ell\right] \tag{4.17}$$

We have already argued heuristically that the method is second order accurate in time as long as $\lambda^2 << \Delta t_k$ holds. This will be verified numerically in Sec. 6. For actual computations (4.16) and (4.17) are inserted into (4.14) and (4.15) and J_n and J_p are computed after the fact. Given ψ^k, n^k and p^k solving (4.13) - (4.17) amounts to solving 3 coupled P.D.E.'s for ψ^{k+1}, n^{k+1} and p^{k+1} at each timestep which is the same ammount of labor as is required by backward differences at each timestep.

idea: We use backward differences for (4.2) a) and centered differences (the trapezoidal rule) for (4.2) b). So we choose a mesh $0 = t_0 < t_1 < \ldots$ and meshsizes $\Delta t_k := t_{k+1} - t_k$, $k = 0,1, \ldots$ and approximate the gridfunctions (ψ,u,J,J_u) at $t = t_k$ by (ψ^k,u^k,J^k,J_u^k) (4.2) a) - b) is now discretized by:

$$\frac{\lambda^2}{\Delta t_k} \operatorname{div}_h \nabla_h (\psi^{k+1} - \psi^k) = \operatorname{div}_h J^{k+1} \tag{4.7}$$

$$\frac{1}{\Delta t_k} (u^{k+1} - u^k) = \frac{1}{2} [\operatorname{div}_h (J_u^k + J_u^{k+1})] - R^k - R^{k+1} \tag{4.8}$$

$$J^{k+1} = -(Mu^{k+1}) \nabla_h \psi^{k+1} + \kappa^{k+1} [\nabla_h (C + \lambda^2 \operatorname{div}_h \nabla_h \psi)] \tag{4.9}$$

$$J_u^\ell = \kappa^\ell \nabla_h u^\ell - M(C + \lambda^2 \operatorname{div}_h \nabla_h \psi^\ell) \cdot \nabla_h \psi^\ell \tag{4.10}$$

$\ell = k, k + 1$ where

$$R^\ell = R(\nabla_h \psi^\ell, n^\ell, p^\ell), \quad \kappa^\ell = \kappa(\nabla_h \psi^\ell), \quad \ell = k, k + 1 \tag{4.11}$$

holds. The local discretization error L in (4.7) and (4.8) is given by

$$L = (\lambda^2 \Delta t_k \operatorname{div}_h \nabla_h \psi_{tt}, \Delta t_k^2 u_{ttt}) \tag{4.12}$$

Thus $\|L\| \leq \text{const } (\lambda^2 \Delta t_k + \Delta t_k^2)$ holds. Since we aim to use stepsizes $\Delta t_k >> \lambda^2$ $\|L\| = O(\Delta t_k^2)$ holds for all practical purposes. (This is verified numerically in Sec. 6.) For numerical purposes it is inconvenient to actually solve (4.7) -

n, p, J_n, J_p can be recovered by virtue of

$$n = \frac{1}{2}\,(u+\lambda^2\,\mathrm{div}_h\nabla_h\psi + C) \quad , \quad p = \frac{1}{2}\,(u-\lambda^2\,\mathrm{div}_h\nabla_h\psi - C)$$

(4.5)

$$J_n = \frac{1}{2}\,(J + J_u) \quad , \quad J_p = \frac{1}{2}\,(J - J_u)$$

the boundary conditions (3.17) have to be transformed appropriately. In this form it is clear that (4.2) a) together with (4.3) constitutes the fast time scale component while (4.2) b) together with (4.4) constitutes the slow time scale component. Inserting (4.3) into (4.2) a) gives in leading order

$$\lambda^2\,\mathrm{div}_h\nabla_h\psi_t = -\mathrm{div}_h[(Mu)\nabla_h\psi] + \ldots. \tag{4.6}$$

which is the discrete equivalent of (2.12). Since u = n + p will be positive and bounded away from zero throughout most of the device ψ can evolve on the timescale $\tau = t/\lambda^2$.

On the other hand u apparently evolves on the ('slow') t-time-scale only (which also is the scale on which the applied voltage V in (0.9) is varied. We therefor employ a strategy which has been successfully employed by Kreiss and Nichols [1975] and Ringhofer [1984] a). That is to use lower order, onesided, A-stable schemes for the fast components of the system and to use symmetric schemes for the 'slow' components which are of higher order but only A-stable. It can in general be expected, that the strong stability properties of the A-stable method can be retained while its lower order accuracy does not destroy the overall accuracy. We restrict ourselves to the simplest version of this

4. Discretization in Time

We now derive a discretization scheme for the system of ordinary differential equations (3.14) - (3.16). It turns out that second order methods based on centered differencing (i.e. the trapezoidal rule or the box-scheme) experience severe stability problems. This is due to the presence of several different time scales in the analytical problem (1.5) - (1.7) (see Sec. 2). So the O.D.E. system (3.14) - (3.16) is stiff. In order to circumvent this problem (3.14) - (3.16) is transformed into an equivalent system which allows the separation into a 'fast' and a 'slow' component. For the fast component we use an L-stable 1st order method (i.e. backward differences). For the slow component we use an A-stable 2nd order method (i.e. the trapezoidal rule). This will avoid any restrictions on the timesteps. On the other hand it is well known that in such a situation the use of a lower order method for the fast component does not destroy the over all (second order) accuracy of the scheme precisely because of the stiffness (see c.f. Ringhofer [1984] a). So we obtain a second order method which does not suffer from prohibitive timestep restrictions. In order to separate the fast and the slow components of (3.14) - (3.16) we differentiate (3.14) with respect to t and introduce the new variables

$$(4.1) \qquad u = n + p,\ J = J_n + J_p,\ J_u = J_n - J_p$$

we obtain

$$(4.2) \qquad a)\ \lambda^2\, \mathrm{div}_h\, \nabla_h \psi_t = \mathrm{div}_h\, J \quad ,\quad b)\ u_t = \mathrm{div}_h J_u - 2R$$

$$(4.3) \qquad J = -(Mu)\nabla_h \psi + \kappa \nabla_h C + \lambda^2 \kappa \nabla_h\, \mathrm{div}_h\, \nabla_h \psi$$

$$(4.4) \qquad J_u = \kappa \nabla_h u - (MC)\nabla_h \psi - \lambda^2 (M\, \mathrm{div}_h\, \nabla_h \psi)\nabla_h \psi$$

(3.16) (a) $J_n = [\kappa \nabla_h n - (Mn)\nabla_h \Psi]$

(3.16) (b) $J_p = -[\kappa \nabla_h p + (Mp)\nabla_h \Psi]$

for $(x_i, y_j) \in G_I$

(3.17) $B(\Psi, n, p, \nabla_h \Psi, J_n, J_p) = 0$ for $x_i, y_j) \in G_B$.

Thus we have replaced the mixed parabolic-elliptic system (1.5) - (1.7) by the ODE system (3.15) - (3.16) coupled to the algebraic system (3.14). The scope of the next section will be to discretize (3.14) - (3.16) in time by a L-stable second order finite difference scheme.

The fitting factor matrix κ is a function of $\nabla_h \psi$ and is given by

$$\kappa_{ij} = \begin{matrix} \sigma(\psi_{i+1j} - \psi_{ij}) & 0 \\ 0 & \sigma(\psi_{ij+1} - \psi_{ij}) \end{matrix} \tag{3.11}$$

$$\sigma(z) := \frac{z}{2} (e^z + 1)(e^z - 1)^{-1} \tag{3.12}$$

The discretization (3.8) - (3.9) can be motivated in the following way:

For a certain set of boundary conditions (corresponding to the equilibrium case) J_n and J_p will vanish identically and n and p will be of the form

$$n = Ae^{\psi} \quad , \quad p = Ae^{-\psi} \tag{3.13}$$

for some constant A. In this case (1.7) a), b) is solved exactly by (3.8) - (3.9). In Markowich Ringhofer et al [1983] a singular perturbation analysis of the steady state problem has been carried out and it has been shown that κ in (3.11) is precisely the correct fitting factor if (1.5) - (1.7) is viewed in the framework of exponentially fitted schemes for singularly perturbed problems (see c.f. Doolan et.al. [1980]. (3.6) - (3.7) together with (3.8) - (3.9) together with the boundary conditions (0.7) now give the discretization of (1.5) - (1.7):

$$\lambda^2 \, \mathrm{div}_h \, \nabla_h \psi = n - p - C \tag{3.14}$$

$$a) \ \frac{\partial}{\partial t} n = \mathrm{div}_h \, J_n + R \quad , \quad b) \ \frac{\partial}{\partial t} p = -\mathrm{div}_h \, J_p + R \tag{3.15}$$

discretized by centered differences in a straightforward manner

$$\lambda^2 \, \mathrm{div}_h \, \nabla_h \psi = n - p - C \tag{3.6}$$

$$\text{a)} \ \frac{\partial}{\partial t} n = \mathrm{div}_h J_n - R \quad , \quad \text{b)} \ \frac{\partial}{\partial t} p = -\mathrm{div}_h J_p - R \tag{3.7}$$

$$(x_i, y_j) \in G_I$$

where $R_{ij} = R(n_{ij} p_{ij})$ holds. It is the current relations (1.7) a), b) which have to be discretized with care. As mentioned in the previous section layers can be expected to occur in ψ, n and p across the p-n-junction (where $C(x,y)$ changes its sign rapidly). Markowich and Ringhofer et.al. [1983] point out that a mesh which equidistributes the local discretization error will inevitably contain a prohibitive ammount of points if the p-n-junction does not lie parallel to the gridline directions (which can not be expected in general). Scharfetter and Gummel [1969] suggested the following discretization of (1.7) a), b):

$$J_n = [\kappa \nabla_h n - (\mathfrak{M} n) \cdot \nabla_h \psi] \tag{3.8}$$

$$J_p = -[\kappa \nabla_h p + (\mathfrak{M} p) \nabla_h \psi] \tag{3.9}$$

where the matrix operator $\mathfrak{M}$ is defined by

$$(\mathfrak{M} u)_{ij} \ \frac{1}{2} \begin{pmatrix} u_{i+1j} + u_{ij} & 0 \\ 0 & u_{ij+1} + u_{ij} \end{pmatrix} \quad u = n, p \tag{3.10}$$

$$(3.3) \qquad J_s = (J_s^x, J_s^y)^T \quad , \quad J_s^x\left(\frac{x_i + x_{i+1}}{2}, y_j, t\right) \sim J^x_{s\,i+1/2,j}(t)$$

$$J_s^y\left(x_i, \frac{y_j + y_{j+1}}{2}\right) \sim J^y_{s\,i,j+1/2}(t), \quad s = n,p.$$

In order to write the discrete approximations of the spacial differential operators in (1.5) - (1.7) in a convenient form we introduce the following difference operators: For a vectorfield $\vec{v}$ given on the intermediate points of the grid G we define the discrete divergence operator by

$$(3.4) \qquad \mathrm{div}_h \vec{v}_{ij} := 2(\delta x_i + \delta x_{i-1})^{-1}(v^x_{i+1/2,j} - v^x_{i-1/2,j}) +$$

$$2(\delta y_j + \delta y_{j-1})^{-1}(v^y_{i,j+1/2} - v^y_{i,j-1/2}) \quad \text{where}$$

$$\vec{v}_{ij} = (v^x_{i+1/2,j}, v^y_{i,j+1/2}) \quad \text{holds}$$

for a scalar gridfunction u we define the discrete gradiend ∇_h by

$$(3.5) \qquad \nabla_h u_{ij} := (d^x_h u_{i+1/2,j}, d^y_h u_{i,j+1/2})^T,$$

$$d^x_h u_{i+1/2,j} := \delta x_i^{-1}(u_{i+1,j} - u_{ij})$$

$$d^y_h u_{i,j+1/2} := \delta y_j^{-1}(u_{i,j+1} - u_{ij}).$$

Poisson's equation (1.5) and the continuity equations (1.6) a), b) are now

3. Spacial Discretization

In this section we discuss the discretization of (1.5) - (1.7) in the spacial variable $\vec{x}$ leaving the time t continuous. Thus (1.5) - (1.7) is replaced by a large sparse system of ordinary differential equations. We utilize an exponentially fitted finite difference scheme due to Scharfetter and Gummel [1969] which has been widely used for the solution of the steady state problem (2.8) - (2.10). First we choose a nonuniform but rectangular mesh in space:

(3.1) $G = \{(x_i, y_j),\ i = 0(1)N,\ j = 0(1)M\}$ with

$$0 = x_0 < x_1 < \ldots < x_N = 1$$

$$0 = y_0 < y_1 < \ldots < y_M = d$$

$$\delta x_i := x_{i+1} - x_i,\ i = 0(1)N-1, \quad \delta y_j = y_{j+1} - y_j,\ j = 0(1)M - 1$$

For obvious reasons it is convenient to distinguish between boundary and interior points. So we define

(3.2) $G_I := \{(x_i, y_j),\ \ i = 1(1)N - 1,\ \ j = 1(1)M - 1\},\ \ G_B = G - G_I$

Ψ, n and p are approximated by their values at the gridpoints (x_i, y_j)

$$w(x_i, y_j, t) \sim w_{ij}(t) \qquad w = \Psi, n, p,$$

The current densities J_n and J_p are approximated at the midpoints between two gridpoints

in leading order

$$(2.12) \qquad \Delta\Psi_\tau = -(n+p)\Delta\Psi + \lambda^2\Delta^2\Psi + \ell.o.t.$$

$$\tau = t/\lambda^2$$

In Ringhofer [1984] b) a complete asymptotic expansion of the solution w on the fast timescale $\tau = t/\lambda^2$ is given in the case of 1 space dimension. It turns out that only Ψ and the drift currents $-n\nabla\Psi$, $-p\nabla\Psi$ can evolve on the fast timescale while n and p can only evolve on the 'slow' t-timescale.

(2.8) $\lambda^2 \Delta \Psi = n - p - C$

(2.9) a) $\nabla \cdot J_n = R$, b) $\nabla \cdot J_p = -R$

(2.10) a) $J_n = \nabla n - n \nabla \Psi$, b) $\nabla \cdot J_p = -\nabla p - p \nabla \Psi$

In Ringhofer [1984] b) it is shown that each time (2.7) is violated the solution w will evolve on an additional 'fast' timescale t/λ^2 which corresponds to the dielectric relaxation time in unscaled form. This is of importance for the numerical solution of (1.5) - (1.7) because it means that the problem is stiff in time and special stability (i.e. L - stability) properties will be required of discretization methods. In Ringhofer [1984] b) an asymptotic expansion for the solution on all timescales and for general initial functions has been carried out. We only briefly sketch the results here: It is beneficial to transform the system (1.5) - (1.7): Differentiating (1.5) with respect to time yields

(2.11) $\lambda^2 \Delta \Psi_t = \nabla \cdot (J_n + J_p)$

(2.11) states the conservation of the total current consisting of the drift and diffusion current for electrons and holes $(J_n + J_n)$ and of the displacement current $-\lambda^2 \nabla \Psi_t$. It is well known that the displacement current can evolve on the timescale of the dielectic relaxation time. Whenever $\nabla \cdot [J_n + J_p] \neq O(\lambda^2)$ holds away from the p-n-junction, where $\Delta \Psi$ is bounded for $\lambda \to 0$, Ψ will evolve on the timescale t/λ^2. Inserting the expressions for J_n and J_p from (1.7) gives

(6.1) b) $\Psi(x,t) = \Psi_{b_i}(x) - \frac{1}{2}u(t)$ $\dot{x}$ at the cathode

We simulate a switch from u = 0 (equilibrium) to u = -0.5V (forward bias) in a timeinterval of 10^{-9} sec which corresponds to 0.1 in our scaling. For the recombination rate the Shockly Read Hall - recombination term

$$(6.2) \qquad R = \frac{n.p - n_i^2}{\tau_n(n+n_i) + \tau_p(p+n_i)}$$

has been used. (n_i, τ_n and τ_p are given constants.) The nonlinear system of equations for $(\Psi^{k+1}, n^{k+1}, p^{k+1})$ arising in (4.13) - (4.17) at each timestep has been solved by Newton's method using a damping strategy due to Deuflhard [1974]. The purpose of this testexample is twofold: Firstly it should verify the stability properties mentioned in Sec. 4, i.e. we should observe that no oscillations occur if $\Delta t_k >> \lambda^2$ is chosen at any point in time. Secondly it should verify the second order accuracy in time. Therefor a fixed mesh is chosen in the spacial direction and it is verified numerically how well the system of ordinary differential equations (3.14) - (3.16) is approximated by (4.13) - (4.17) by varying the timesteps Δt_k. So we choose a rectangluar nonuniform grid

$$(6.3) \qquad G : \{(x_i, y_j) \quad , \quad i = 0(1)n \quad , \quad j = 0(1)m\}$$

where the gridlines are clustered around the p-n-junction. The maximal mesh spacing has been chosen as

$$\overline{\delta x} := \max\{\delta x_i : \delta x_i = x_{i+1} - x_i,\ i = 0(1)n - 1\} = 0.05$$

(6)

$$\overline{\delta y} := \max\{\delta y_j : \delta y_j = y_{j+1} - y_j,\ j = 0(1)m - 1\} = 0.05$$

Then a solution is computed on a quite course mesh in time which is obtained by bounding the growth in the drift - and diffusion current density: i.e.

$$\|J^{k+1} - J^k\|_2 \leq w\|J^k\|_2$$

(6.5)

$$J^\ell = J_n^\ell + J_p^\ell \quad , \quad \ell = k,\ k + 1$$

is required at each step with some suitable parameter w. (Here $\|\cdot\|_2$ denotes the discrete L_2-norm.) Using this strategy the coarsest mesh

(6.6) $$T_0 := \{t_i^0 : i = 0(1)K\}$$

is obtained. Then the meshspacings are halved successively to obtain the meshes $T_1, T_2 \ldots$:

(6.7) $$T_\ell := \{t_i^\ell : i = 0(1)2^\ell K\} \quad , \quad \ell =$$

$$t_i^\ell = \begin{cases} t_j^{\ell-1} & , \ i = 2j \\ \frac{1}{2}(t_{j+1}^{\ell-1} + t_j^{\ell-1}) & , \ i = 2j + 1 \end{cases}$$

Then the solution on the finest mesh is regarded as 'exact' solution and the relative differences (in the discrete L_2 norm) to the coarser-mesh solutions are computed. If the method is of second order they should decay asymptotically by a factor 4 from T_ℓ to $T_{\ell+1}$. Table 1 gives the relative errors in the L_2 norm:

TABLE 1

ℓ	PSI	N	P	$J = J_n + J_p$	JP
0	0.33E-01	0.89E+00	0.15E+00	0.58E+00	0.39E+00
1	0.10E-01	0.17E+00	0.46E-01	0.18E+00	0.12E+00
2	0.16E-02	0.27E-01	0.74E-02	0.29E-01	0.20E-01
3	0.17E-03	0.62E-02	0.77E-03	0.31E-02	0.20E-02
4	0.39E-04	0.16E-02	0.18E-03	0.80E-03	0.45E-03
5	0.84E-05	0.38E-03	0.38E-04	0.21E-03	0.94E-04

As a test (3.14) - (3.16) has been solved on the same meshes in the spacial and the time direction by using the same spacial discretization but simple backward differences for n_t and p_t in (3.15) a) b). The relative differences to the finest-grid-solutions for this case should decay by a factor 2 from T_ℓ to $T_{\ell+1}$ because of the first order accuracy. They are given in Table 2:

TABLE 2

ℓ	PSI	N	P	$J = J_n + J_p$	JP
0	0.11E-01	0.13E+01	0.52E-01	0.20E+00	0.14E+00
1	0.67E-02	0.75E+00	0.30E-01	0.12E+00	0.83E-01
2	0.37E-02	0.39E+00	0.17E-01	0.64E-01	0.45E-01
3	0.19E-02	0.19E+00	0.83E-02	0.32E-01	0.23E-01
4	0.81E-03	0.83E-01	0.37E-02	0.14E-01	0.10E-01
5	0.25E-03	0.28E-01	0.12E-02	0.48E-02	0.34E-02

Comparing Tables 1 and 2 it can also be seen that to compute c.f. $J = J_n + J_p$ with a relative accuracy of 1% 4 times as many timesteps are required by backward differences shown by the proposed method. In Figures 1 - 9 plots of the solution at various time levels. The switch from u = 0.v to v 0.5v is performed in the interval from t = 0.1 to t = 0.2.

Figure 1 shows the initial solution $\psi(\vec{x},0)$ which has been taken as the steady state solution for u = 0.v (equilibrium).

Figures 2 - 8 show the solution at t = 0.2 (the end of the switching interval). In particular they show

Figure 2: $\psi(\vec{x},0.2)$

Figure 3: $n(\vec{x},0.2)$

Figure 4: $p(\vec{x}, 0.2)$

Figures 5 and 6: The x and y components of

$$J_n(\vec{x},0.2)$$

Figures 7 and 8: the x and y components of

$$J_p(\vec{x},0.2)$$

Figure 9 shows the total current flow through the cathode contact as a function of time:

$$J_{T_0 t}(t) = \int_{\text{cathode}} (-\nabla\psi_t + J_n + J_p) \cdot \vec{n}\, ds$$

where n is the normal vector to the cathode.

FIGURE 1 (PSI)

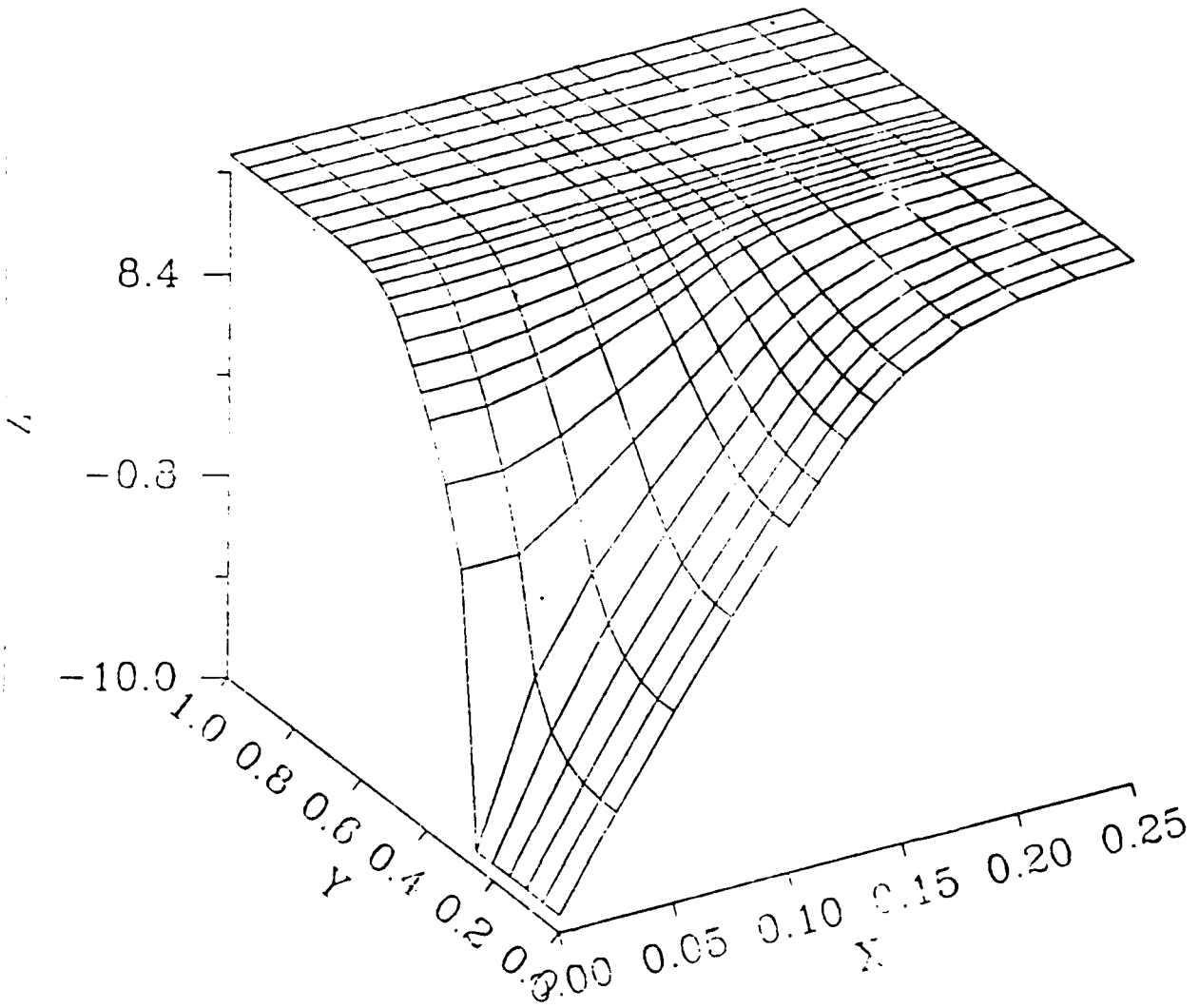


FIGURE 2 (PSI)

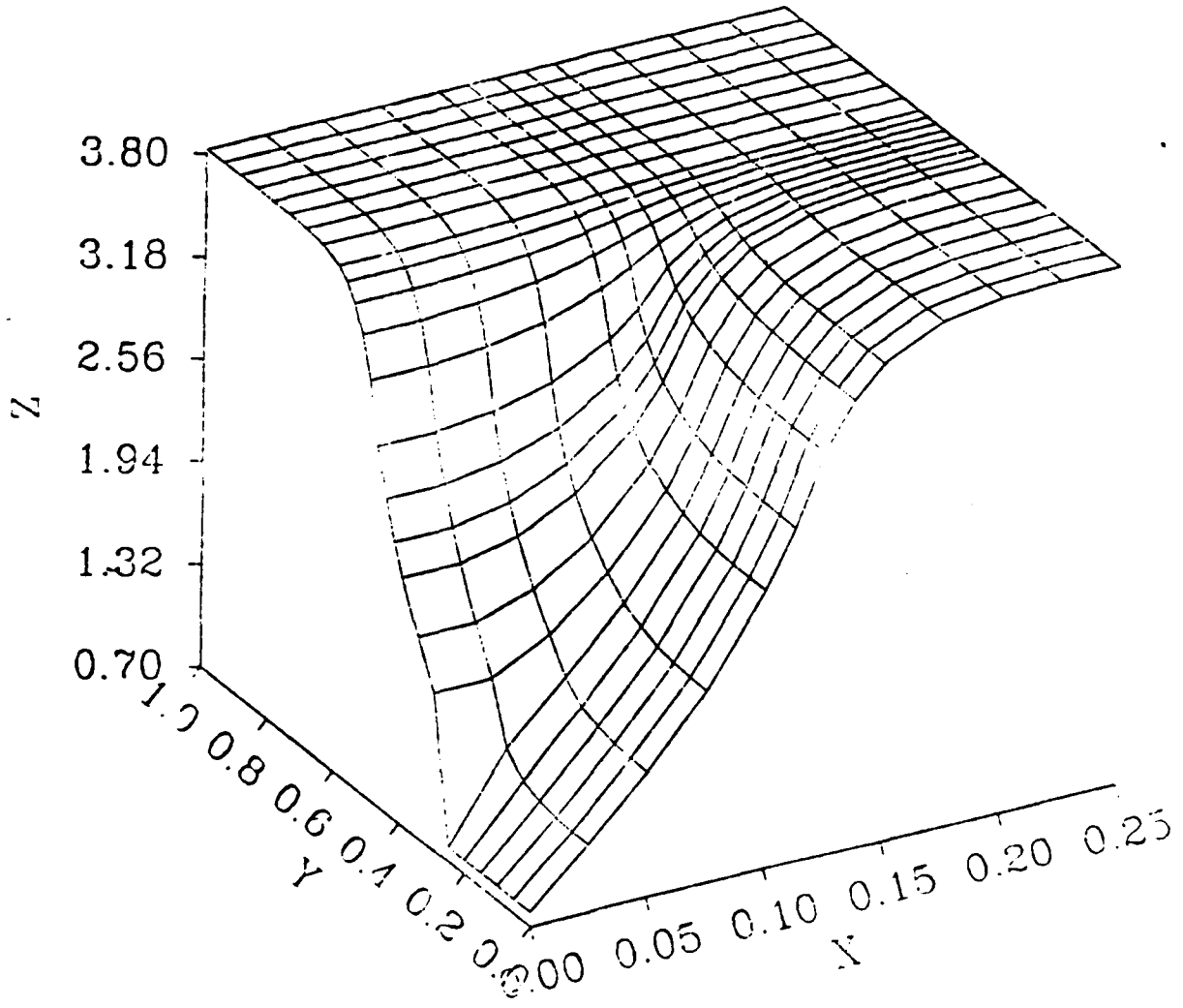

3.80
3.18
2.56
1.94
1.32
0.70
Z
1.0 0.8 0.6 0.4 0.2 0.0
Y
0.00 0.05 0.10 0.15 0.20 0.25
X

FIGURE 3 (N)

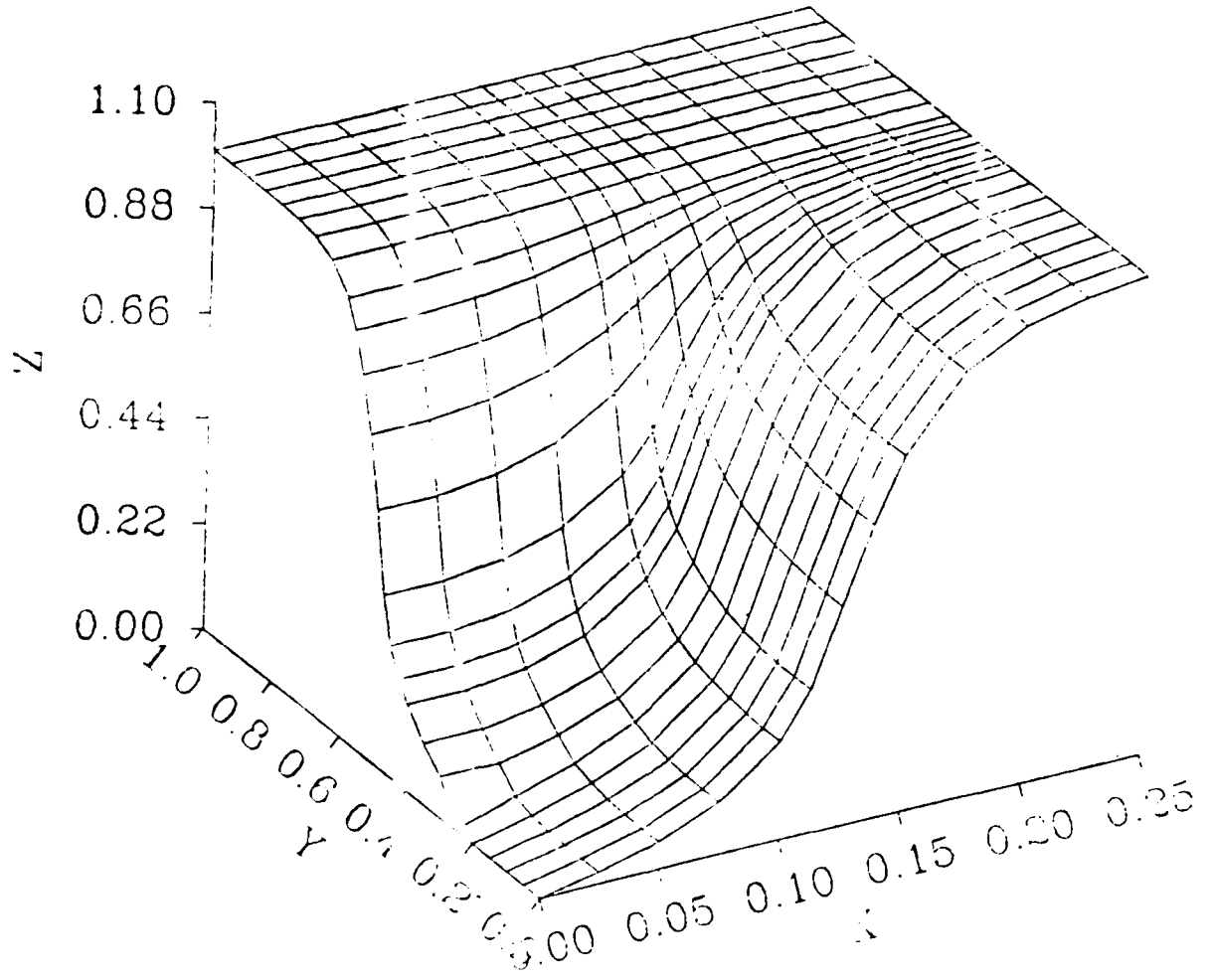


FIGURE - (P)

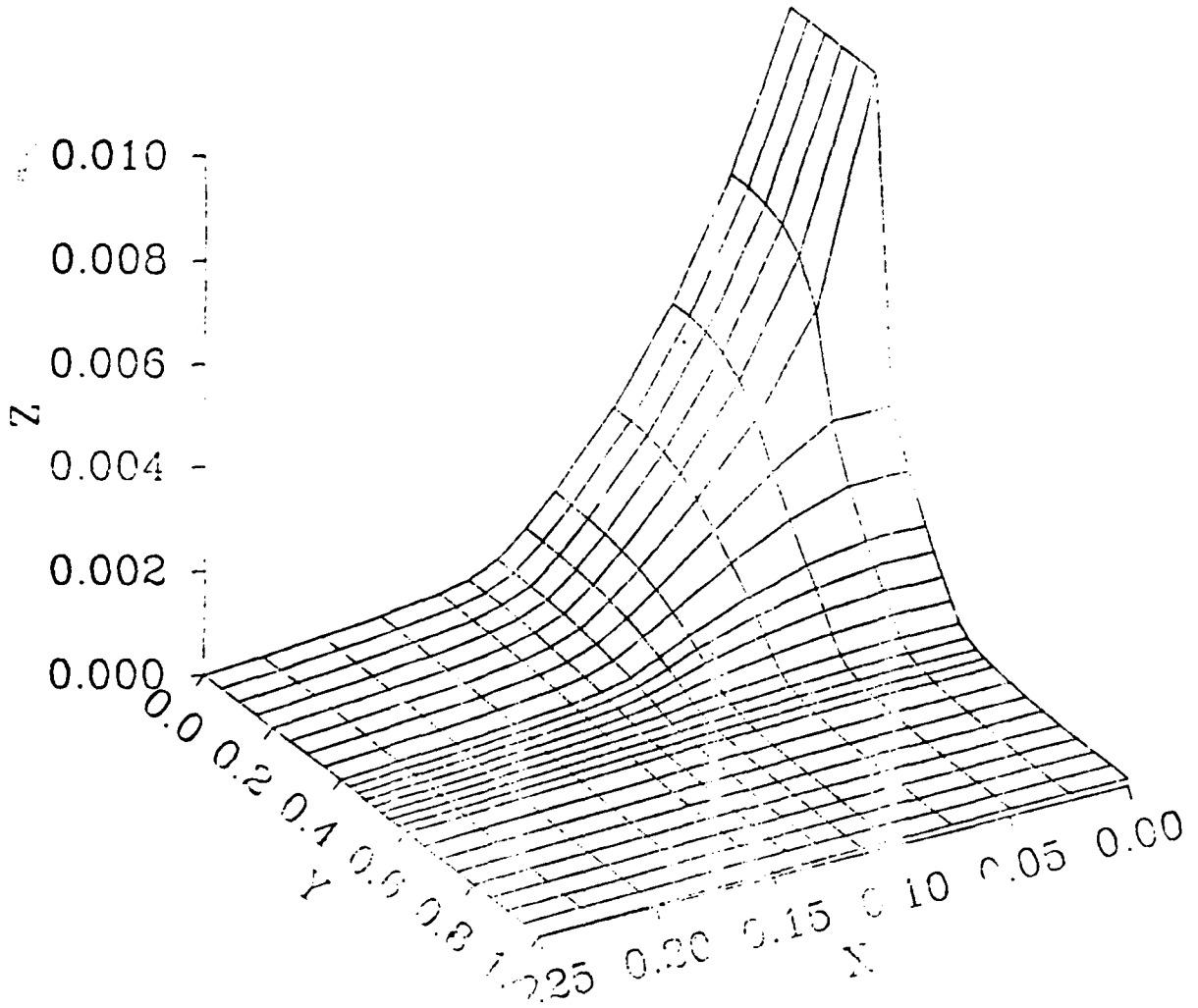


FIGURE 5 (JMY)

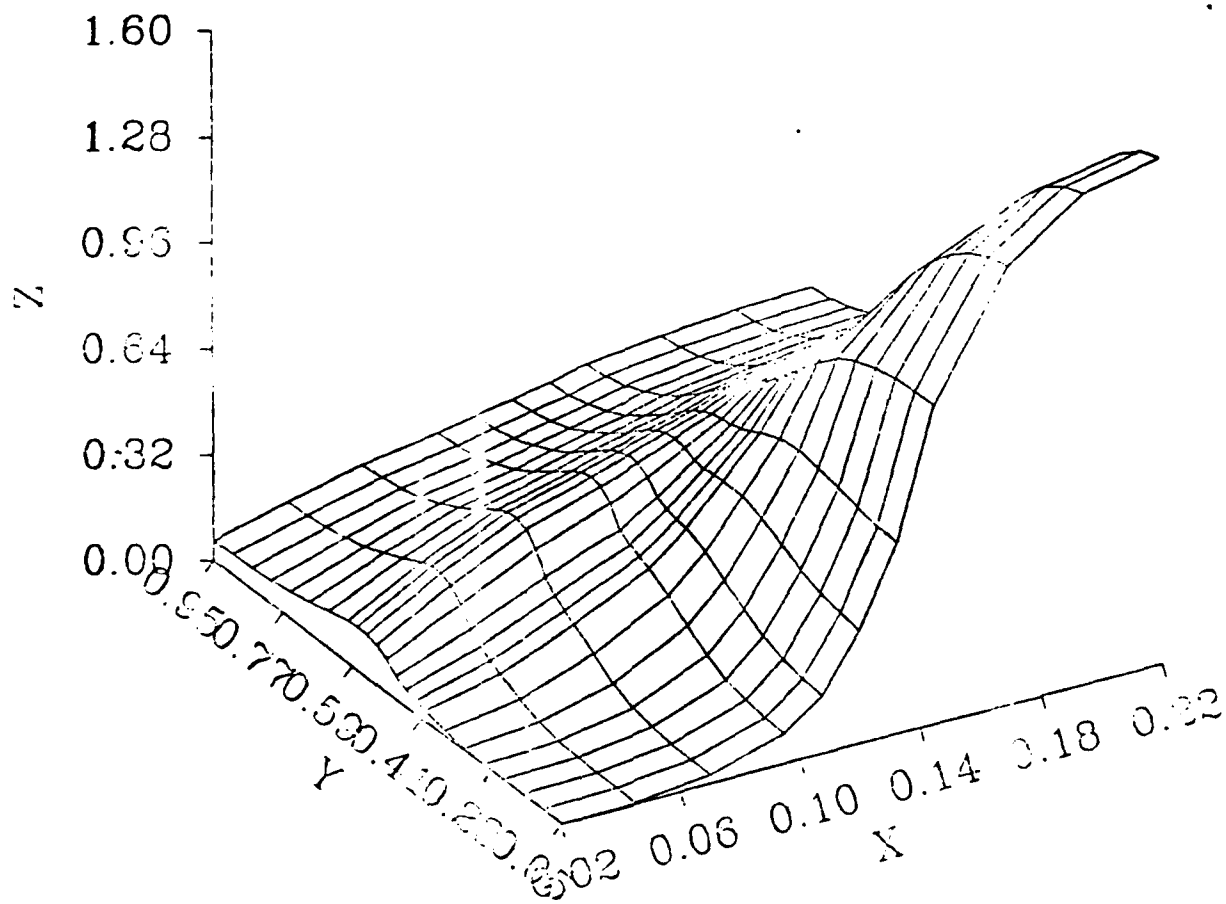


FIGURE 6 (M,Y)

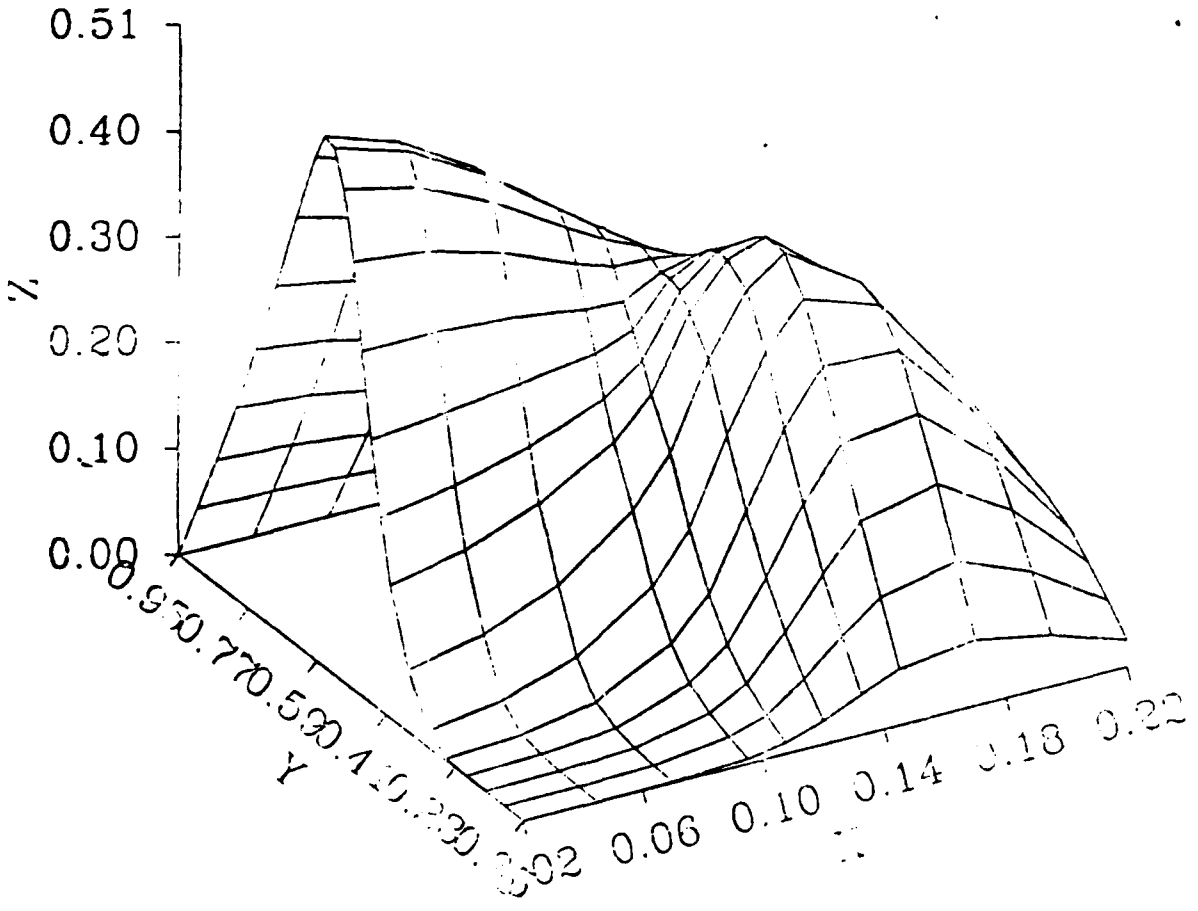


FIGURE 7 (JPX)

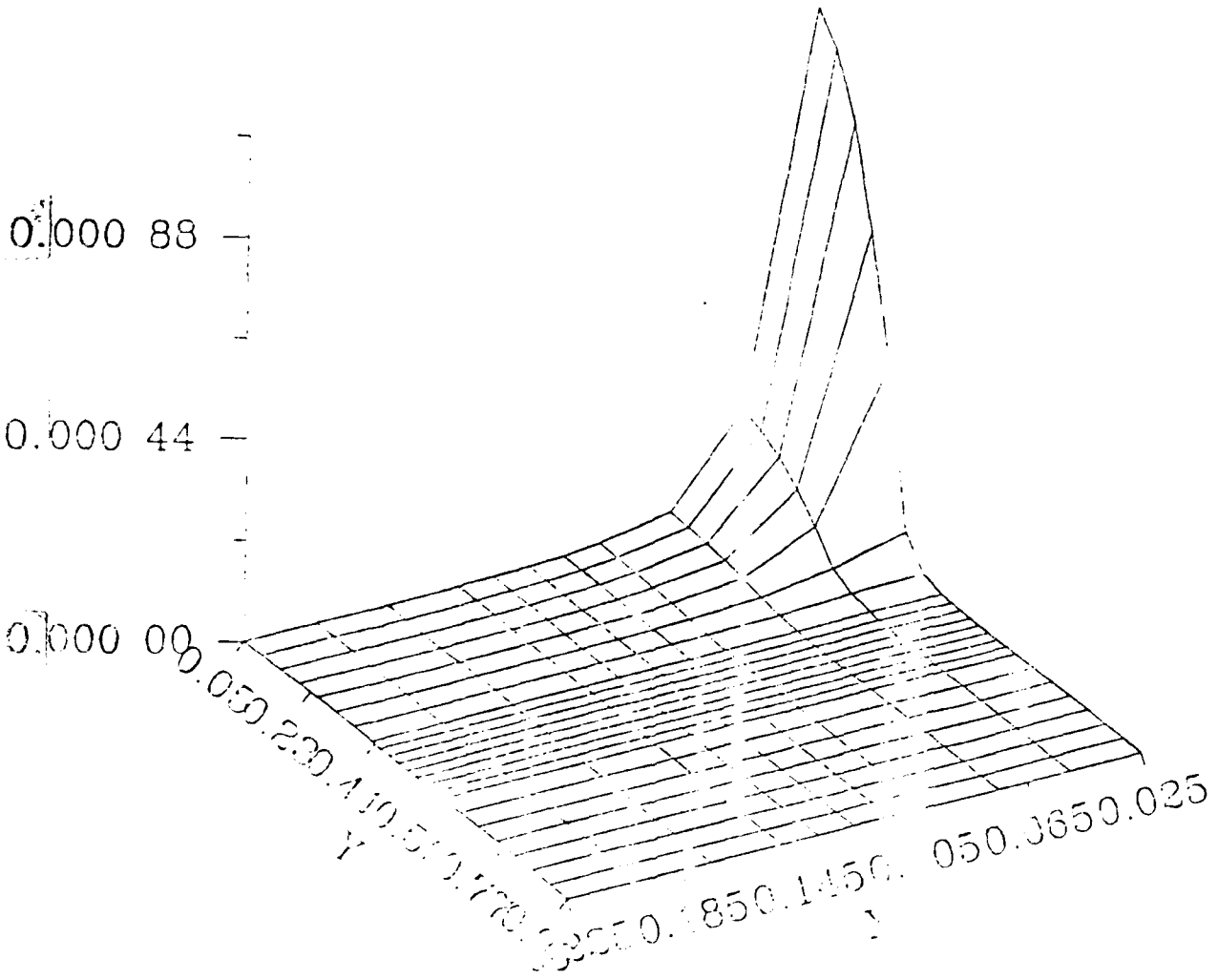
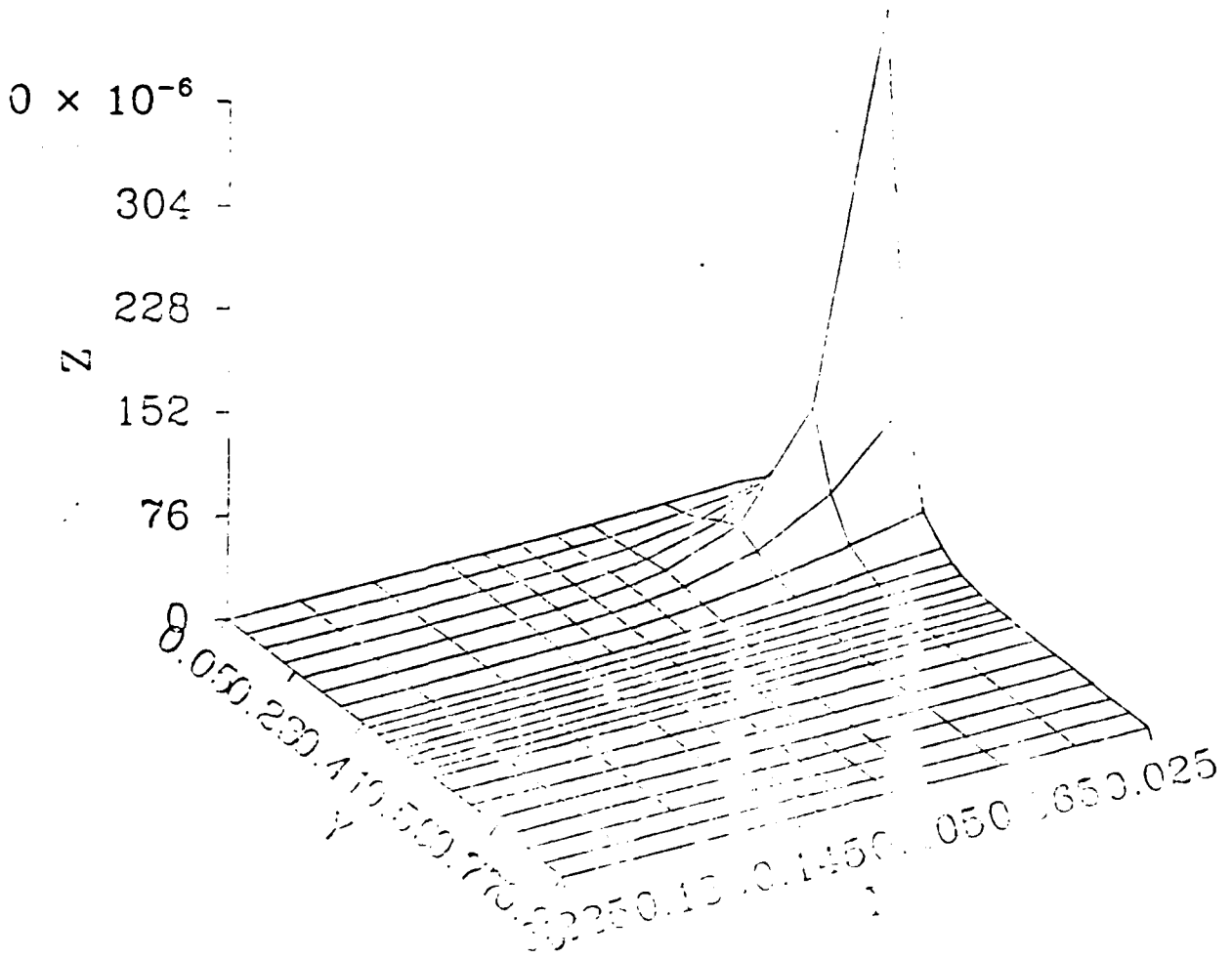


FIGURE 3 (HPY)



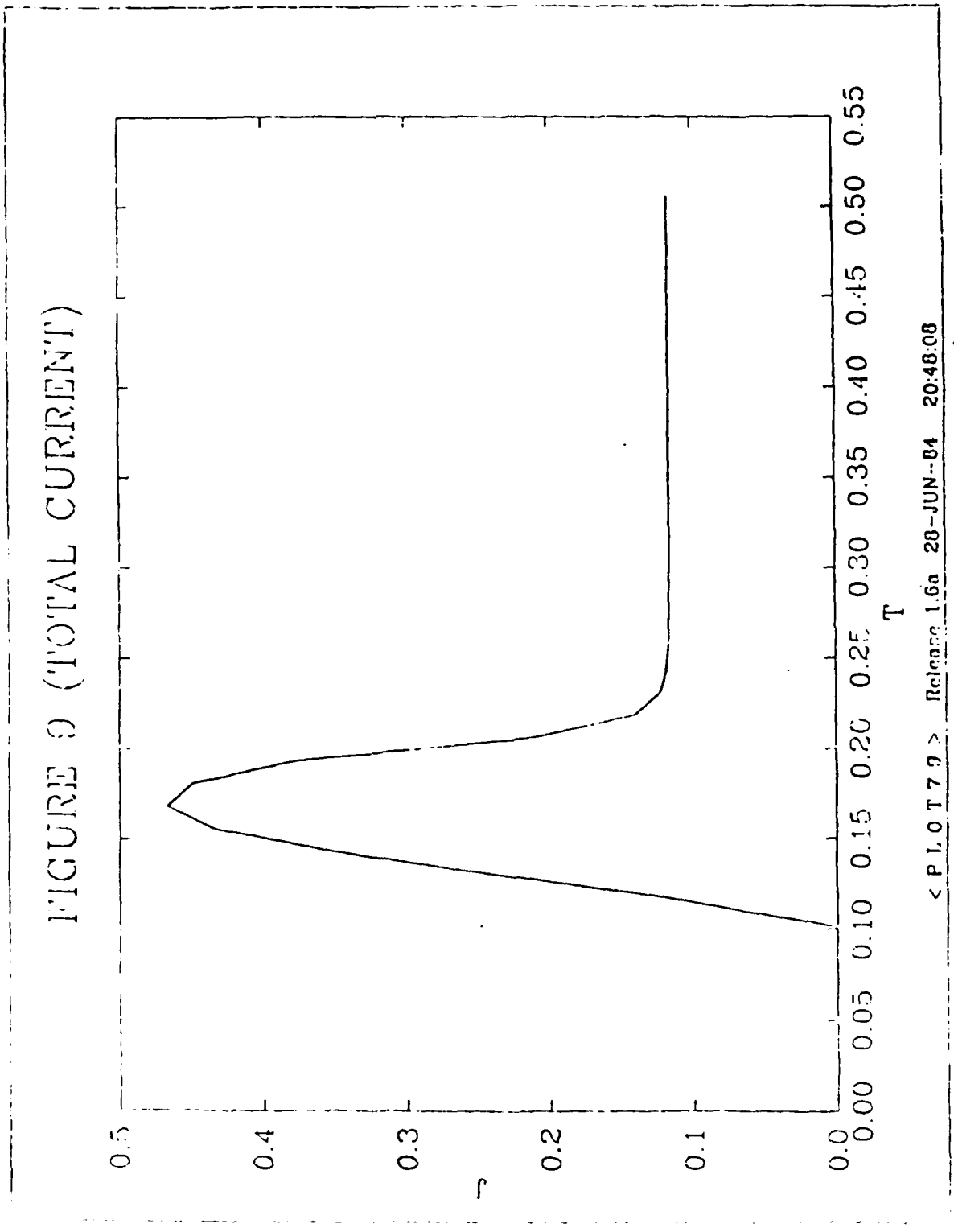


FIGURE 9 (TOTAL CURRENT)
0.5
0.4
0.3
0.2
0.1
0.0
I
0.00 0.05 0.10 0.15 0.20 0.25 0.30 0.35 0.40 0.45 0.50 0.55
T
< P L O T 7 9 > Release 1.6a 28-JUN-84 20:48:08

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A second order scheme for the solution of the transient fundamental semiconductor device equations is presented which does not suffer from timestep restrictions due to the stiffness of the analytical problem. The second order accuracy as well as the stability properties are demonstrated on the simulation of a p-n-junction diode.

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